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- X-ray spectroscopy*
- Splitting of the $1s^{-1}3p$ resonance in sulfur K XANES by surroundings in compounds with sulfur-carbon double bond, K.-H. Hallmeier, A.A. Pavlychev, R. Szargan, L. Beyer, C. Hennig and F. Thiel 178 (1993) 349
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- A 2+1 REMPI study of the E-X transition in CO. Indirect predissociations in the E $^1\Pi$ state, J. Baker, J.L. Lemaire, S. Couris, A. Vient, D. Malmasson and F. Rostas 178 (1993) 569

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- Radiative lifetimes of the $A\ ^2\Sigma_{1/2}^+$ and $X_2\ ^2\Pi_{3/2}$ states of lead monohalides, O. Shestakov, H. Demes and E.H. Fink 178 (1993) 561

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- Theoretical studies of the electronic spectrum of SiF_2 , Z.-L. Cai and J.-L. Bai 178 (1993) 215

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- Laser excitation and emission spectroscopy of the methoxy radical in a supersonic jet, P. Misra, X. Zhu, C.-Y. Hsueh and J.B. Halpern 178 (1993) 377
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-neat

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- Structural relaxation in amorphous biphenyl and a new crystalline phase, H. Nakayama, M. Kawahara and K. Ishii 178 (1993) 371

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- Numerical application of the coupled cluster theory with localized orbitals to polymers. I. Total correlation energy per unit cell, Y.-J. Ye, W. Förner and J. Ladik 178 (1993) 1
- Disordered polaron transport: a theoretical description of the motion of photoinjected charges in molecularly doped polymers, D.H. Dunlap and V.M. Kenkre 178 (1993) 67
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- Small angle X-ray scattering and viscoelastic studies of the molecular shape and colloidal structure of bovine and rat serum albumins in aqueous systems, T. Matsumoto and H. Inoue 178 (1993) 591

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- Ro-vibronic spectrum of the N_2O^+ ion in the $X^2\Pi$ state, H. Gritli, Z.B. Lakhdar, G. Chambaud and P. Rosmus 178 (1993) 223

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- Radiative lifetimes of the $A^2\Sigma_{1/2}^+$ and $X_2^2\Pi_{3/2}$ states of lead monohalides, O. Shestakov, H. Demes and E.H. Fink 178 (1993) 561
- A 2+1 REMPI study of the E-X transition in CO. Indirect predissociations in the $E^1\Pi$ state, J. Baker, J.L. Lemaire, S. Couris, A. Vient, D. Malmasson and F. Rostas 178 (1993) 569

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- The electronic spectrum of carbon dioxide. Discrete and continuum photoabsorption oscillator strengths (6–203 eV), W.F. Chan, G. Cooper and C.E. Brion 178 (1993) 401
- Study of isotope effects in the ground state of the symmetrical isotopomers of CuCl_2 , P. Crozet, J.C. Coste, R. Bacis, A.J. Bouvier, S. Churassy and A.J. Ross 178 (1993) 505
- Singlet state energy levels of $\text{C}_2\text{H}_4^{2+}$ by double charge transfer spectroscopy, P.G. Fournier, J. Fournier, M.L. Langford and F.M. Harris 178 (1993) 581
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Free radicals (including hydronium and muonium)

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- The Green function method in the theory of nuclear and electron spin polarization. I. General theory, zero approximation and applications, P.A. Purtov and A.B. Doktorov 178 (1993) 47
- Statistical simulation of IF angle and angle-velocity distributions from the crossed beam reaction $F + I_2 \rightarrow IF + I$, P.-A. Elofson and L. Holmlid 178 (1993) 315
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- Are there geometric isomers of the van der Waals dimers $Ar-OCS$ and $Ar-SO_2$?, R.G.A. Bone 178 (1993) 255
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- Laser excitation and emission spectroscopy of the methoxy radical in a supersonic jet, P. Misra, X. Zhu, C.-Y. Hsueh and J.B. Halpern 178 (1993) 377
- Normal modes of 4-aminobenzonitrile (4-ABN). A comparison of PM3 calculations with experimental jet-cooled spectroscopy, H. Yu, E. Joslin, S.M. Zain, H. Rzepa and D. Phillips 178 (1993) 483
- Study of isotope effects in the ground state of the symmetrical isotopomers of $CuCl_2$, P. Crozet, J.C. Coste, R. Bacis, A.J. Bouvier, S. Churassy and A.J. Ross 178 (1993) 505
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- Scaled ab initio force field of E- and Z-hexatriene in the S_0 and T_1 states, F. Negri, G. Orlandi, F. Zerbetto, P. Palmieri and R. Tarroni 178 (1993) 133
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- Valence electronic structure of a long-chain alkane in random-coil forms. Gas-phase UPS of $n\text{-C}_{36}\text{H}_{74}$ and MO calculations, K. Seki, N. Sato and H. Inokuchi 178 (1993) 207
- Theoretical studies of the electronic spectrum of SiF_2 , Z.-L. Cai and J.-L. Bai 178 (1993) 215
- Ro-vibronic spectrum of the N_2O^+ ion in the $X^2\Pi$ state, H. Gritli, Z.B. Lakhdar, G. Chambaud and P. Rosmus 178 (1993) 223
- Splitting of the $1s^{-1}3p$ resonance in sulfur K XANES by surroundings in compounds with sulfur-carbon double bond, K.-H. Hallmeier, A.A. Pavlychev, R. Szargan, L. Beyer, C. Hennig and F. Thiel 178 (1993) 349
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- Time-resolved LIF spectroscopy on $\text{N}_2(\text{A})$ metastable in a He/ N_2 pulsed rf discharge, S. De Benedictis, G. Dilecce and M. Simek 178 (1993) 547

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- Potential energy surfaces of ozone in its ground state and in the lowest-lying eight excited states, A. Banichevich, S.D. Peyerimhoff and F. Grein 178 (1993) 155
- Excited-state intramolecular proton transfer in jet-cooled 1-hydroxy-2-acetonaphthone, A. Douhal, F. Lahmani and A. Zehnacker-Rentien 178 (1993) 493

Luminescence spectra, yields and lifetimes

- Fluorescence lifetime measurements and hole-burning experiments on J-aggregates of a benzimidocarbocyanine dye, M. Lindrum, A. Glismann, J. Moll and S. Daehne 178 (1993) 423
- Radiative lifetimes of the $\text{A } ^2\Sigma_{1/2}^+$ and $\text{X}_2 \text{ } ^2\Pi_{3/2}$ states of lead monohalides, O. Shestakov, H. Demes and E.H. Fink 178 (1993) 561

Multiphoton phenomena

- A 2+1 REMPI study of the E–X transition in CO. Indirect predissociations in the $\text{E } ^1\Pi$ state, J. Baker, J.L. Lemaire, S. Couris, A. Vient, D. Malmasson and F. Rostas 178 (1993) 569

Reactions (including dissociation)

- The Green function method in the theory of nuclear and electron spin polarization. I. General theory, zero approximation and applications, P.A. Purtov and A.B. Doktorov 178 (1993) 47

- Statistical simulation of IF angle and angle-velocity distributions from the crossed beam reaction $F + I_2 \rightarrow IF + I$, P.-A. Elofson and L. Holmlid 178 (1993) 315
- Ground- and lowest excited-state MRDCI potential-energy surfaces for the collinear $Li + HF$ reaction, C. Suárez, A. Aguado and M. Paniagua 178 (1993) 357
- gas phase*
- Effective core potential study of transition metal and lanthanide catalyzed hydrogen exchange, T.R. Cundari, W.J. Stevens and S.O. Sommerer 178 (1993) 235
- Theoretical calculations of the quartet potential energy surfaces in the $NH^+ + H_2$ system, R. Polák, I. Paidarová and P.J. Kuntz 178 (1993) 245
- Theoretical study of the lowest potential energy surfaces for the reaction $O(^3P) + HBr(X^1\Sigma^+) \rightarrow OH(X^2\Pi) + Br(^2P)$, J. Urban and V. Staemmler 178 (1993) 279
- A quasiclassical trajectory study of the effect of the initial rovibrational level and relative translational energy of reactants on the dynamics of the $N(^4S_u) + O_2(X^3\Sigma_g^-) \rightarrow NO(X^2\Pi) + O(^3P_g)$ atmospheric reaction on the $^2A'$ ground potential energy surface, M. Gilibert, A. Aguilar, M. González and R. Sayós 178 (1993) 287
- A detailed SACM study of the $H + NO \rightarrow HNO$ reaction based on a realistic potential energy surface, C.J. Cobos 178 (1993) 329
- Ground- and lowest excited-state MRDCI potential-energy surfaces for the collinear $Li + HF$ reaction, C. Suárez, A. Aguado and M. Paniagua 178 (1993) 357
- photochemical*
- Measurement of very long (10^7 s) spin conversion times: dimethyl-s-tetrazine in durene, M. Joyeux, B. Prass, C. von Borczyskowski, J.-C. Vial and H.P. Trommsdorff 178 (1993) 433
- Excited-state intramolecular proton transfer in jet-cooled 1-hydroxy-2-acetonaphthone, A. Douhal, F. Lahmani and A. Zehnacker-Rentien 178 (1993) 493
- Tunneling*
- A detailed SACM study of the $H + NO \rightarrow HNO$ reaction based on a realistic potential energy surface, C.J. Cobos 178 (1993) 329
- Electron transfer*
- Disordered polaron transport: a theoretical description of the motion of photoinjected charges in molecularly doped polymers, D.H. Dunlap and V.M. Kenkre 178 (1993) 67
- Time resolution of ion pair formation in poly(N-vinylcarbazole), S. Nešpůrek 178 (1993) 415
- Singlet state energy levels of $C_2H_4^+$ by double charge transfer spectroscopy, P.G. Fournier, J. Fournier, M.L. Langford and F.M. Harris 178 (1993) 581
- Ionization (including Rydberg states)*
- The electronic spectrum of water in the discrete and continuum regions. Absolute optical oscillator strengths for photoabsorption (6–200 eV), W.F. Chan, G. Cooper and C.E. Brion 178 (1993) 387
- The electronic spectrum of carbon dioxide. Discrete and continuum photoabsorption oscillator strengths (6–203 eV), W.F. Chan, G. Cooper and C.E. Brion 178 (1993) 401
- Singlet state energy levels of $C_2H_4^+$ by double charge transfer spectroscopy, P.G. Fournier, J. Fournier, M.L. Langford and F.M. Harris 178 (1993) 581

Molecular motion (including diffusive)

- Molecular dynamics simulation of the plastic phase of 2-methyl-2-nitropropane, S. Labate, G. Cardini, R. Righini and S. Califano 178 (1993) 93

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- Study of isotope effects in the ground state of the symmetrical isotopomers of CuCl_2 , P. Crozet, J.C. Coste, R. Bacis, A.J. Bouvier, S. Churassy and A.J. Ross 178 (1993) 505

Surface effects and catalysis

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- Structural phase transitions and orientational ordering in C_{70} , G.B.M. Vaughan, P.A. Heiney, D.E. Cox, J.E. Fischer, A.R. McGhie, A.L. Smith, R.M. Strongin, M.A. Cichy and A.B. Smith III 178 (1993) 599